

Approximate analytical solutions for arbitrary l -state of the Hulthén potential with an improved approximation of the centrifugal term

Research Article

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Abstract: An approximate analytical solution of the radial Schrödinger equation for the generalized Hulthén potential is obtained by applying an improved approximation of the centrifugal term. The bound state energy eigenvalues and the normalized eigenfunctions are given in terms of hypergeometric polynomials. The results for arbitrary quantum numbers n_r and l with different values of the screening parameter δ are compared with those obtained by the numerical method, asymptotic iteration, the Nikiforov-Uvarov method, the exact quantization rule, and variational methods. The results obtained by the method proposed in this work are in a good agreement with those obtained by other approximate methods.

Keywords: Hulthén potential • Energy eigenvalues and eigenfunctions • Centrifugal term

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1. Introduction

The search for exact solutions of the radial Schrödinger equation (SE) in some physical potential models has been an important research area since the birth of quantum mechanics. Unfortunately, the rigorous solutions are known only for a few simple cases. One of the reasons for the lack of explicit expression for the eigenfunctions and energy eigenstates is the presence of the centrifugal term $1/r^2$ in the corresponding SE. The Hulthén potential is here a good example. The radial SE has an exact solution only for the states with zero angular momentum. Since its introduction in 1942 [1] quite a lot of methods [2] have been developed to find a rigorous solution for $l = 0$ states. However, when the centrifugal term is taken into account, the corresponding SE can no longer be solved in a closed form and it is necessary to resort to approximate methods. Over the last few decades several schemes have been used to calculate the energy spectrum. The main idea of these schemes relies on using different approximations of the centrifugal term. In 1976 Greene and Aldrich [3] have proposed a method for approximating the centrifugal term by means of $1/r^2 \approx \delta^2 e^{-\delta r} / (1 - e^{-\delta r})^2$. Using their approximation scheme some authors obtained analytically the arbitrary l -wave bound [4] and scattering states [5]

of the Hulthén potential. However, it should be noted that this approximation is valid only for small values of the screening parameter δ . For large values of δ it breaks down leading to substantial errors in energy eigenvalues. A new approximation scheme for the centrifugal term in the form $1/r^2 \approx \delta^2 [\omega v(r) + v^2(r)]$ has been proposed by Jia *et al.* [6], where $v(r) = e^{-\delta r} / (1 - e^{-\delta r})$, and ω is an adjustable parameter. Their results are in good agreement with those obtained by other methods but also in the small screening δ regime. Recently Ikhdair [7] proposed an alternative approximation scheme based on the expansion of the centrifugal term in a series of exponentials depending on the internuclear separation r and keeping terms up to second order $1/r^2 \approx \delta^2 [d_0 + v(r) + v^2(r)]$, where d_0 is the shifting parameter. Although the differences in both approximations are small the energy spectrum obtained by Ikhdair coincides better with those obtained by numerical integration, especially for high screening δ values.

It is worth mentioning here that apart from different approximation schemes, a variety of analytical methods have been developed to find the expressions for the energy eigenvalues and the wave functions in a closed form. Aguilera-Navarro *et al.* [8] investigated this potential using variational methods. The Nikiforov-

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Uvarov (NU) method has been applied in Ikhdair and Sever paper [9], and the asymptotic iteration method (AIM) in Bayrak *et al.* paper [10]. Gönül *et al.* [11] used a supersymmetric quantum mechanics method. By using exact quantization rule (EQR) Qiang *et al.* [4d] have developed another alternative method. Finally, Tang and Chan [12] proposed in their letter the shifted $1/N$ expansion method. All results obtained by these methods have been compared with those obtained by other approximate methods and the energy spectra together with the radial wavefunction have been given in an explicit and closed form.

The aim of this work is to give an analytical solution of the Hulthén potential using an improved approximation scheme of the centrifugal term proposed by Badawi *et al.* [13]. Their method is based on the use of the centrifugal term in a form formally homogeneous to the original potential to keep the factorizability of the corresponding SE. Taking the centrifugal term as

$$\frac{1}{\delta^2 r^2} = \frac{1}{x^2} = c_0 + \frac{c_1 e^{-x}}{1 - e^{-x}} + \frac{c_2 e^{-2x}}{(1 - e^{-x})^2}, \quad (1)$$

where C_i parameters can be determined as a function of the specific potential parameters, they showed that direct factorization becomes possible for potentials like Morse-Pekeris, Rosen-Morse, Manning-Rosen or Tietz. The same scheme has been used by Lu [14] or Ikhdair and Sever [15] for the empirical potential introduced by Schiöberg [16]. As we mentioned above, a similar expansion has been applied for Hulthén potential by Jia and collaborators [6] but with ω taken as an adjustable parameter. The expansion (Eq. 1) has been also applied by Ikhdair and Sever [17] to the Manning-Rosen potential.

Although Eq. 1 has proved its power and efficiency when compared with Greene and Aldrich approximation, it does not always lead to the solution in a closed form. For the Hulthén potential considered here we propose a modified approximation scheme similar to this introduced by Lu [14] but where the C_i coefficients are to be determined as a function of the potential parameter depending on the quantum state considered. In order to get these coefficients we start with finding the l -dependent minimum of the effective potential by solving numerically a transcendental equation $dV_{\text{eff}}(r)/dr = 0$. Next, by expanding a new exponential variable in a Taylor's series about l -dependent minimum, truncating this series after the second term and comparing it with Eq. 1 we obtain the l -dependent C_i parameters. Using expansion (Eq. 1) for given C_i parameters we solve the corresponding SE in terms of the generalized hypergeometric function.

In order to verify the accuracy of our approximation scheme, the results are compared with those obtained by numerical integration [18], NU [7], quasi-analytical (QA) [6], EQR [4d] and AIM [10] methods published within the last few years.

The rest of this paper is organized as follows. In the next section we present the bound state solutions and the normalized radial wave functions of the Hulthén potential with an improved approximation of the centrifugal term. In section 3 our results are presented and compared with those of numerical integration and those obtained by the other methods. Finally, in section 4 we give some concluding remarks.

2. Bound state solutions of the Hulthén potential for arbitrary l -states

The Hulthén potential we examine in this paper is defined as $V_H(r) = -Ze^2 \frac{\delta e^{-\delta r}}{1 - e^{-\delta r}}$, where Z , e and δ are the atomic number, electric charge and the screening parameter, respectively. The radial part of the Schrödinger equation for the relative motion of two particles interacting via Hulthén potential can be written as

$$\left[-\frac{\hbar^2}{2\mu} \left(\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} \right) + V_{\text{eff}}(r) \right] R(r) = E R(r), \quad (2)$$

where μ is the reduced mass and the $V_{\text{eff}}(r)$ is the effective potential, which is defined as the sum of the generalized Hulthén potential $V_H(r)$ and the centrifugal term $V_C(r) = \frac{l(l+1)\hbar^2}{2\mu r^2}$ depending on the quantum number l .

Making the standard change $R(r) = r^{-1} u(r)$ and inserting it into Eq. 2 we obtain

$$\left[-\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + V_{\text{eff}}(r) \right] u(r) = E u(r). \quad (3)$$

Because Eq. 3 cannot be solved analytically due to the centrifugal term, we have to use a proper approximation of this term. Unlike the common approximation used for the first time in Greene and Aldrich work, here we applied an improved approximation Scheme 1. Insertion of Eq. 1 and the generalized Hulthén potential $V_H(r)$ into Eq. 3 allows us to obtain

$$\left[-\frac{\hbar^2 \delta^2}{2\mu} \frac{d^2}{dx^2} + V_{\text{eff}}(x) \right] u(x) = E u(x), \quad (4)$$

where

$$V_{\text{eff}}(x) = -Zq^2 \frac{\delta e^{-x}}{1 - e^{-x}} + \frac{l(l+1)\hbar^2 \delta^2}{2\mu} \left[c_0 + \frac{c_1 e^{-x}}{1 - e^{-x}} + \frac{c_2 e^{-2x}}{(1 - e^{-x})^2} \right] \quad (5)$$

and where $x = \delta r$ is a dimensionless variable.

As we will show, Eq. 5 is integrable under the exchange of variables $z = e^{-x}$. After introducing this

new variable we can rearrange Eq. 5 as

$$z^2 \frac{d^2 u(z)}{dz^2} + z \frac{du(z)}{dz} + \left[\frac{\alpha z}{1-z} - \frac{l(l+1)c_2 z^2 + c_2}{(1-z)^2} - \lambda^2 \right] u(z) = 0, \quad (6)$$

where we used the dimensionless parameters given by

$$\lambda^2 = -\frac{2\mu E}{\hbar^2 \delta^2} + l(l+1)c_0, \quad \alpha = \frac{2\mu Z e^2}{\hbar^2 \delta} - l(l+1)c_1. \quad (7)$$

Considering the boundary conditions and bearing in mind that Eq. 6 has two regular singularities at $z=0$ and $z=1$, we take the trial solution of Eq. 6 in the form

$$u(z) = z^\lambda (1-z)^\beta f(z). \quad (8)$$

By substituting Eq. 8 into Eq. 6 we get the following second-order homogeneous differential equation

$$z(1-z) \frac{d^2 f(z)}{dz^2} + [-(2\lambda+2\beta+1)z+2\lambda+1] \frac{df(z)}{dz} + [\alpha - (2\lambda+1)\beta] f(z) = 0, \quad (9)$$

only when we make the following choice for

$$\beta = \frac{1}{2} \sqrt{1+4l(l+1)c_2} + \frac{1}{2}. \quad (10)$$

Eq. 9 corresponds to the well-known hypergeometric equation

$$z(1-z) \frac{d^2 f(z)}{dz^2} + [-(a+b+1)z+c] \frac{df(z)}{dz} - ab f(z) = 0 \quad (11)$$

whose solution is the generalized hypergeometric function [19]

$$f(z) = C_1 \cdot {}_2F_1(a, b; c; z) + C_2 \cdot z^{1-c} {}_2F_1(a - c + 1, b - c + 1; 2 - c; z). \quad (12)$$

By comparing Eq. 11 with Eq. 9 we can immediately write the parameters in Eq. 11 as

$$a = \lambda + \beta - \sqrt{\alpha + \lambda^2 + \beta^2 - \beta} \quad (13a)$$

$$b = \lambda + \beta + \sqrt{\alpha + \lambda^2 + \beta^2 - \beta} \quad (13b)$$

$$c = 1 + 2\lambda. \quad (13c)$$

Considering the boundary condition, i.e., $f(z)$ tending to finite value when $z \rightarrow 0$, the allowed solution is

$$f(z) = C_1 \cdot {}_2F_1(a, b; c; z) = \sum_{k=0}^{\infty} \frac{(a)_k (b)_k}{(c)_k} \frac{z^k}{k!}, \quad (14)$$

where $(a)_k = \frac{\Gamma(a+k)}{\Gamma(a)}$ denotes the Pochhammer symbol. To avoid a divergent behaviour of the hypergeometric series in Eq. 14, the function $f(z)$ must be reduced to a polynomial of degree n_r . It can be accomplished by restricting the values of the parameter $a = -n_r$, where $n_r = 0, 1, 2, \dots$, which leads to a finite series expansion

in Eq. 14 for $k = 0, 1, 2, \dots, n_r$. Substitution of Eq. 13a into $a = -n_r$ gives us the allowed energy spectra for the Hulthén potential $\lambda^2 = (n_r + \lambda + \beta)^2 - \alpha + \beta - \beta^2$, which can be further written as

$$E_{n_r, l} = -\frac{\hbar^2 \delta^2}{2\mu} \left[\frac{(\beta - \alpha + \beta + n_r^2 + 2\beta n_r)^2}{(n_r + \beta)^2} - l(l+1)c_0 \right] \quad (15)$$

with the aid of Eq. 7.

Using $\lambda + \beta - \sqrt{\alpha + \lambda^2 + \beta^2 - \beta} = -n_r$ we can rewrite Eq. 13b as $b = 2\lambda + 2\beta + n_r$, and hence the general solution of Eq. 6 as follows

$$u_{n_r, l}(z) = N_{n_r, l} z^\lambda (1-z)^\beta {}_2F_1(-n_r, 2\lambda + 2\beta + n_r; 1 + 2\lambda; z), \quad (16)$$

where $N_{n_r, l}$ is the normalization constant. This constant can be calculated from the normalization condition

$$\delta^{-1} \int_0^1 |u(z)|^2 \frac{dz}{z} = 1. \quad (17)$$

Putting the wave function of Eq. 16 into Eq. 17 and using the following formula [20]

$$\begin{aligned} & \int_0^1 z^{2\lambda-1} (1-z)^{2\beta} [{}_2F_1(-n_r, 2\lambda + 2\beta + n_r; 1 + 2\lambda; z)]^2 dz \\ &= \frac{(n_r + \beta) \Gamma(n_r + 1) \Gamma(n_r + 2\beta) \Gamma(2\lambda) \Gamma(2\lambda + 1)}{(n_r + \lambda + \beta) \Gamma(n_r + 2\lambda + 1) \Gamma(2\lambda + 2\beta + n_r)}, \end{aligned} \quad (18)$$

we can obtain the analytical expression of normalization constant

$$N_{n_r, l} = \left[\frac{\delta (n_r + \lambda + \beta) \Gamma(n_r + 2\lambda + 1) \Gamma(2\lambda + 2\beta + n_r)}{(n_r + \beta) \Gamma(n_r + 1) \Gamma(n_r + 2\beta) \Gamma(2\lambda) \Gamma(2\lambda + 1)} \right]^{1/2}. \quad (19)$$

Before we use Eq. 15 to get the energy eigenvalues we have to obtain the coefficients c_0 , c_1 and c_2 . Following the well-known approach we can treat these coefficients as an adjustable parameters. However here, we will show how to get them as a function of the specific potential parameters. We start with rewriting the equation $z = e^{-x}$ as

$$\frac{1}{x^2} = \frac{1}{\ln(z)^2} = \frac{1}{\ln(z_l + \Delta z)^2}, \quad (20)$$

where $\Delta z = z - z_l$, and z_l is the l -dependent minimum of $V_{\text{eff}}(z_l)$.

Bearing in mind that the energy eigenvalues are mainly determined by the behaviour of the effective potential in the region near the l -dependent minimum, we expand the centrifugal term in Eq. 20 around the l -dependent minimum. It is obvious that for the effective potential considered here we can get only approximate z_l by solving numerically the following equation $dV_{\text{eff}}(r)/dr = 0$. Hence, expanding the right-hand side of Eq. 20 in a series around $\Delta z = 0$ to the second order we get

Table 1. The bound state energy eigenvalues ($-E_n$) of the Hulthén potential as a function the screening parameter δ for 2p, 3p,3d, 4p, 4d, 4f, 5p, 5d, 5f, 5g, 6p, 6d, 6f and 6g states in atomic units ($\hbar = m = e = 1$) and $Z = 1$.

State	δ	Present	Numerical [18]	NU [7]	QA. [6]	EQR [4d]	AIM [10]
2p	0.025	0.1127604	0.1127605	0.1127611	0.1126344	0.1128125	0.1128125
	0.05	0.1010420	0.1010425	0.1010442	0.1009128	0.1012500	0.1012500
	0.075	0.0898453	0.0898478	0.0898495	0.0898350	0.0903125	0.0903125
	0.1	0.0791717	0.0791794	0.0791769	0.0794011	0.0800000	0.0800000
	0.15	0.0594007	0.0594415	0.0593981	0.0604650	0.0612500	0.0612500
	0.2	0.0417491	0.0418860	0.0417078	0.0441045	0.0450000	0.0450000
	0.25	0.0262466	0.0266111	0.0261059	0.0303195	0.0312500	0.0312500
	0.3	0.0129347	0.0137900	0.0125925	0.0191101	0.0200000	0.0200000
	0.35	0.0018698	0.0037931	0.0011675	0.0104763	0.0112500	0.0112500
3p	0.025	0.0437066	0.0437069	0.0437072	0.0436848	0.0437590	0.0437590
	0.05	0.0331602	0.0331645	0.0331623	0.0332390	0.0333681	0.0333681
	0.075	0.0239173	0.0239397	0.0239207	0.0242183	0.0243837	0.0243837
	0.1	0.0159798	0.0160537	0.0159825	0.0166227	0.0168056	0.0168056
	0.15	0.0040316	0.0044663	0.0040162	0.0057067	0.0058681	0.0058681
3d	0.025	0.0436028	0.0436030	0.0436044	0.0435371	0.0437587	0.0437587
	0.05	0.0327495	0.0327532	0.0327508	0.0329817	0.0333681	0.0333681
	0.075	0.0230109	0.0230307	0.0229948	0.0238893	0.0243837	0.0243837
	0.1	0.0144147	0.0144842	0.0143364	0.0162600	0.0168055	0.0168055
	0.15	0.0008528	0.0013966	0.0003124	0.0053907	0.0058681	0.0058681
4p	0.025	0.0199480	0.0199489	0.0199486	0.0199625	0.0200000	0.0200000
	0.05	0.0110422	0.0110582	0.0110442	0.0111938	0.0112500	0.0112500
	0.075	0.0045340	0.0046219	0.0045370	0.0049439	0.0050000	0.0050000
	0.1	0.0004252	0.0007550	0.0004269	0.0012128	0.0012500	0.0012500
4d	0.025	0.0198444	0.0198462	0.0198457	0.0198877	0.0200000	0.0200000
	0.05	0.0106355	0.0106674	0.0106327	0.0110819	0.0112500	0.0112500
	0.075	0.0036479	0.0038345	0.0036111	0.0048327	0.0050000	0.0050000
4f	0.025	0.0196903	0.0196911	0.0196914	0.0197756	0.0200000	0.0200000
	0.05	0.0100463	0.0100620	0.0100154	0.0109150	0.0112500	0.0112500
	0.075	0.0024452	0.0025563	0.0022222	0.0046682	0.0050000	0.0050000
5p	0.025	0.0094011	0.0094036	0.0094017	0.0094325	0.0094531	0.0094531
	0.05	0.0026047	0.0026490	0.0026067	0.0027900	0.0028125	0.0028125
5d	0.025	0.0092977	0.0093037	0.0092988	0.0093914	0.0094531	0.0094531
	0.05	0.0022001	0.0023131	0.0021952	0.0027454	0.0028125	0.0028125
5f	0.025	0.0091451	0.0091521	0.0091445	0.0093298	0.0094531	0.0094531
	0.05	0.0016381	0.0017835	0.0015779	0.0026791	0.0028125	0.0028125
5g	0.025	0.0089441	0.0089465	0.0089387	0.0092480	0.0094531	0.0094531
	0.05	0.0009496	0.0010159	0.0007549	0.0025920	0.0028125	0.0028125
6p	0.025	0.0041493	0.0041548	0.0041500	0.0041899	0.0042014	0.0042014
6d	0.025	0.0040460	0.0040606	0.0040471	0.0041671	0.0042014	0.0042014
6f	0.025	0.0038945	0.0039168	0.0038927	0.0042014	0.0042014	0.0042014
6g	0.025	0.0036996	0.0037201	0.0036870	0.0040876	0.0042014	0.0042014

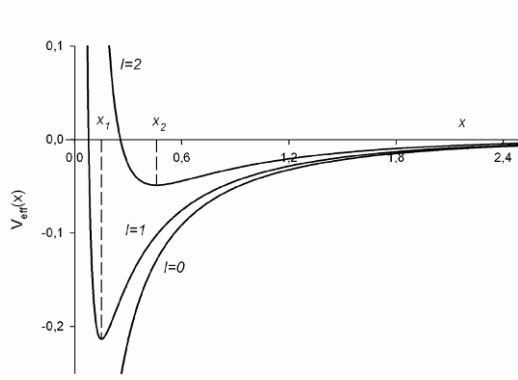


Figure 1. The effective Hulthén potential for $l = 0$, $l = 1$ and $l = 2$ angular momentum quantum numbers. The parameters are in atomic units ($\hbar = m = e = 1$) with $Z = 1$ and $\delta = 0.075$.

$$\frac{1}{x^2} = \frac{1}{\ln(z_l)^2} - \frac{2}{z_l \ln(z_l)^3} \Delta z + \left[\frac{3 + \ln(z_l)}{z_l \ln(z_l)^4} \right] \Delta z^2 + O(\Delta z^3). \quad (21)$$

On the other hand, if we write the approximation from Eq. 1 used for the centrifugal term as

$$\frac{1}{x^2} = c_0 + \frac{c_1(z_l + \Delta z)}{(1 - z_l - \Delta z)} + \frac{c_2(z_l + \Delta z)^2}{(1 - z_l + \Delta z)^2}, \quad (22)$$

and expand it also in a Taylor series around $\Delta z = 0$ to the second order we get

$$\begin{aligned} \frac{1}{x^2} = c_0 + \frac{c_1 z_l}{1 - z_l} + \frac{c_2 z_l^2}{(1 - z_l)^2} + \left[\frac{(2c_2 - c_1)z_l + c_1}{(1 - z_l)^3} \right] \Delta z + \\ + \left[\frac{(2c_2 - c_1)z_l + c_1 + c_2}{(1 - z_l)^4} \right] \Delta z^2 + O(\Delta z^3). \end{aligned} \quad (23)$$

By equating terms of like powers of in Eqs. 21 and 23 we obtain

$$\begin{aligned} c_0 &= \frac{1}{\ln(z_l)^2} - \frac{z_l^2 + 2z_l - 3}{\ln(z_l)^3} + \frac{3z_l^2 - 6z_l + 3}{\ln(z_l)^4} \\ c_1 &= -\frac{2z_l^2 - 6z_l + 4}{z_l \ln(z_l)^3} + \frac{6z_l^3 - 18z_l^2 + 18z_l - 6}{z_l \ln(z_l)^4} \\ c_2 &= -\frac{z_l^4 - 2z_l^3 + 2z_l - 1}{z_l^2 \ln(z_l)^3} + \frac{3z_l^4 - 12z_l^3 + 18z_l^2 - 12z_l + 3}{z_l^2 \ln(z_l)^4}. \end{aligned} \quad (24)$$

3. Results and Discussion

To proceed with our improved approximation scheme we start with plotting the effective potential $V_{\text{eff}}(x)$ for different angular momentum quantum numbers l . As shown in Fig. 1, the minimum point of $V_{\text{eff}}(x)$ for $l = 0$ is a singular point. It exists only for $l \neq 0$ states and it increases considerably as the angular momentum increases. At this same time the well depth decreases

as the angular momentum increases. Because the standard approximation is based on the expansion of the centrifugal term in a series around x_0 , it is obvious that it could be valid only for the potential with a singularity point $x_0 \neq 0$, and accurate for values of x close to x_0 , i.e., for low angular momentum energy states. Here we used the only possible and more accurate form of expansion around l -dependent equilibrium point $x_l \equiv z_l$. Allowing x_l to differ from x_0 we get a significant increase in the accuracy of the resulting expansion, because it allows variation of the equilibrium point for the angular momentum state considered.

To show the accuracy of this approximation scheme, we calculated the energy eigenvalues for arbitrary quantum numbers $n = n_r + l + 1$ and l for different values of the screening parameter δ . The results are given in Table 1 and compared with those obtained by using other methods. As follows from the table, the accuracy of our results is the same or even better than that provided by the other methods. The relative errors $\frac{|E(\text{approx}) - E(\text{num})|}{E(\text{num})}$ for the majority of eigenvalues are less than 1%, and are up to ~10 times better than the best estimations provided by [7] for some eigenvalues.

The differences between various methods become more apparent for large values of δ parameters and appear due to the approximation of the centrifugal term, which simply means that the better the accuracy in calculating energy eigenvalues the better the approximation of the centrifugal term, and hence the whole model.

4. Conclusions

It is well known that the Hulthén potential is one of the important exponential model potential, and it has been a subject of interest in many fields of physics and chemistry. In this work, we have obtained the energy eigenvalues and normalized eigenfunctions of the Hulthén potential using the proposed improved approximation scheme of the centrifugal term. The main results of this paper are the explicit and closed form expressions for the energy eigenvalues and the normalized wave functions. The method presented in this paper is a systematic one and in many cases more accurate than the other ones. As can be expected this approximation scheme can be successfully applied not only for the potential considered here but also for the other exponential-type potentials.

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